MICROWAVE SPECTRA, MOLECULAR STRUCTURE AND AROMATIC CHARACTER OF BN-NAPHTHALENE (4A,8A-AZABORANAPHTHALENE)[a]

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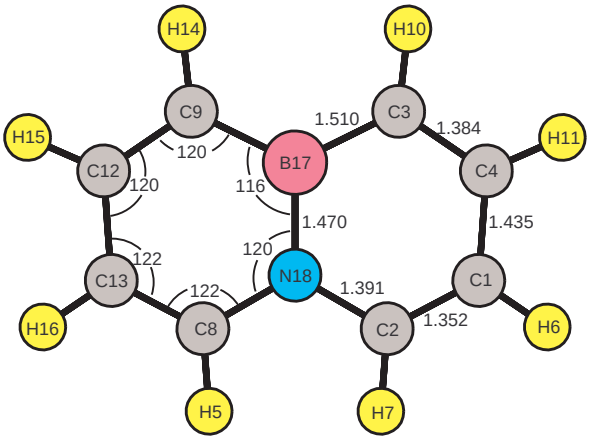
The microwave spectra for seven unique isotopologues of BN-naphthalene (4a,8a-azaboranaphthalene) were measured using a pulsed-beam Fourier transform microwave spectrometer. Spectra were obtained for the normal isotopologues with ^{10}B, ^{11}B, all unique single ^{13}C and the ^{15}N isotopologue, in natural abundance. The rotational, centrifugal distortion and quadrupole coupling constants determined for the ^{11}B^{14}N isotopologue are A = 3042.7128(4) MHz, B = 1202.7066(4) MHz, C = 862.2201(4) MHz, D_J = 0.06(1) kHz, 1.5 eQq_{aa} (^{14}N) = 2.578(6) MHz, 0.25(eQq_{bb}- eQq_{cc}) (^{14}N) = -0.119(2) MHz, 1.5 eQq_{aa} (^{11}B) = -3.922(8) MHz, and 0.25(eQq_{bb}- eQq_{cc}) (^{11}B) = -0.907(2) MHz. The experimental inertial defect is Δ = -0.159 amu Å^2, which is consistent with a planar structure. The B-N bond length is 1.47 Å, indicating π-bonding character. The results are compared with similar results for B-N bonding in 1,2-dihydro-1,2-azaborine and BN-cyclohexene.



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